THE NEIGHBOR SWITCHING MECHANISM OF SUPERPLASTIC DEFORMATION

By

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To the faculty of Washington State University:

The members of the Committee appointed to examine the dissertation of DAVID JOHN SHERWOOD find it satisfactory and recommend that it be accepted.

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Abstract

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At one time the notion that crystal plasticity resulted from the simultaneous motion of lattice planes over one another was entertained. This idea was displaced by the concept that relative atomic motions occur sequentially when dislocations move through the crystal. Similarly, McLean suggested that grains switch neighbors sequentially in a polycrystalline material undergoing superplastic flow. Morral and Ashby observed that the neighbor switching reactions in a froth occurred at irregular cells, and that these irregularities were associated with dislocations in the cellular array. They introduced cellular dislocation glide as a model for superplastic flow, and suggested that if the concentration of these defects required to make the froth flow increased with the flow stress, then the froth would have a non-Newtonian viscosity, like many superplastic materials. Cahn and Padawer pointed out that cellular dislocation climb was used as a model for grain growth by Hillert; this process results in the elimination of cells from the froth. Sato, Kuribayashi and Horiuchi used cellular dislocation climb to model both grain motion and the deformation-enhanced grain growth which can accompany superplastic flow.

Here, the neighbor switching mechanism of superplastic deformation is developed as a topic in dislocation theory.

The compatibility theory of dislocations is developed at an introductory level with exterior calculus. "Compatibility" of a cellular array corresponds to statements, *a la* Rivier, about the distribution of edges amongst the cells. The theory of dislocation motion, or crystal plasticity, is also developed with exterior calculus. Morral and Ashby's constitutive relationship for superplastic flow is analyzed and two models for deformation-enhanced grain growth are developed. The constitutive relationship and grain growth kinetics for superplastic flow are illustrated by modelling the behavior exhibited by single phase (Sn-1% Bi) and quasi-single phase (7475 Al) materials. It is suggested that the grain growth kinetics are strain rate dependent: kinetics in one strain rate regime give way to different kinetics when the strain rate is changed.

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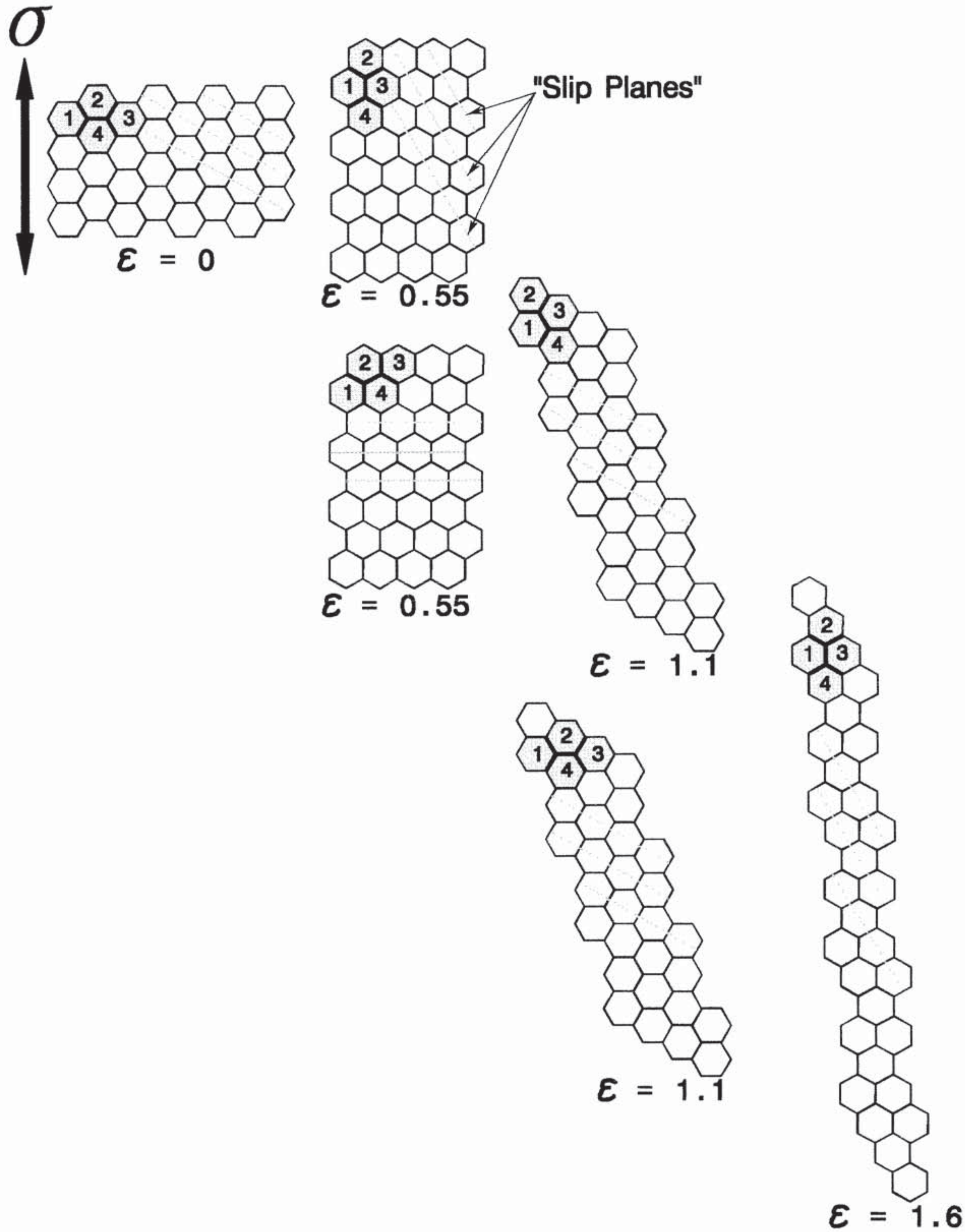
SUMMARY



Most metal alloys are comprised of many distinct crystallites called grains; they are *polycrystalline*. Each grain is a single crystal, separated from the other grains by boundaries. These grain boundaries are "mobile" at temperatures in excess of approximately one-half the melting point of the material; such high temperatures are required to produce creep and superplastic deformation, as well as grain growth. Grain boundaries move by sliding and migrating: Grain boundary sliding induces relative motion of the two grains defined by the boundary, the motion being parallel to the boundary, and can therefore be a type of plastic deformation. Sliding is generally accompanied by grain boundary migration (Ashby 1972). The grain boundary moves normal to itself for grain boundary migration; atoms on one side of the boundary assume the crystallographic orientation of the other. Grain boundary migration does not necessarily involve plastic deformation; it can occur during annealing where the result is grain growth. In a polycrystalline material sliding and/or migrating grain boundaries affect the neighbors of the two grains as well; the neighbor switching mechanism of superplastic deformation (Lee 1970, McLean 1970) accounts for this, as does Hillert's (1965) grain growth "reaction."

Many metals with a small (about ten microns), stable, and equiaxed grain structure, can be deformed superplastically. Very large strains are attainable with superplastic forming because the flow stress has a large strain rate sensitivity, which inhibits necking, and results in great ductility. The grain structure is essentially unaffected by superplastic deformation: grain strain is markedly less than the bulk strain and may even vanish. Material flow occurs because the grains move over and around each other, as opposed to simply stretching as in diffusional and dislocation creep. Such "transilatory grain rearrangements" result in grains being displaced towards the loading direction and away from transverse directions. Grain boundary sliding and migration are required for these rearrangements; the neighbor switching mechanism of superplastic deformation is a model for them.

Grain rearrangements also take place when polycrystalline materials are annealed, where they produce grain growth; but since these rearrangements occur "randomly" they do not redistribute material.

Grain growth tends to occur when metals are subjected to the high temperatures required for superplastic forming. When the grain growth rate increases with increasing strain rate grain growth is being enhanced by the mechanism(s) responsible for superplasticity (Clark and Alden 1973). Too much grain growth limits the formability of superplastic materials: for a given flow stress the strain rate is inversely proportional to the grain size; the strain rate sensitivity decreases with increasing grain size, and material ductility along with it. The influence of grain growth on superplastic forming is, however, rather complex, and in fact it may actually increase ductility in some cases (Hamilton 1989). The effects of deformation-enhanced grain growth and the microstructure's natural tendency to coarsen at the forming temperature are, furthermore, different, because the latter is not dependent on the strain rate.

Understanding the grain growth kinetics of superplastic materials is likely to benefit selection of optimal forming processes (Hamilton 1989). Since these materials are generally complex alloys, *e.g.* quasi-single phase (or particle-containing), their grain growth kinetics are difficult (if not impossible) to accurately predict from first principles. Sherwood and Hamilton (1993) provide an approximation to the grain growth kinetics for quasi-single phase materials by integrating one of Hillert's (1965) grain growth rates.

Data for the grain growth kinetics of a 7475 Al alloy are given in the Appendix. The grain size of this quasi-single phase material is stabilized by a dispersion of small intermetallic particles which inhibit grain boundary migration. Very little grain growth occurs even when this material is annealed at a temperature nearly equal to the melting point. During superplastic deformation the grain growth rate increases with the strain rate, and it also decreases with increasing strain for a given strain rate. For a given strain, the grain size increases with increasing deformation temperature and decreasing strain rate.

Theories of superplastic flow predict that the flow stress varies as a power function of the strain rate, where the exponent of the strain rate, called the strain rate sensitivity (m), is between one-half and one: *flow stress* $\propto$ *strain rate*^{m}. A strain rate sensitivity of at least $m \approx 0.3$ is required for superplastic forming and ductility increases with increasing m. Most theories of superplastic flow predict a single value for this parameter, *e.g.* $m = 0.5$ occurs frequently, yet the strain rate sensitivity changes with the strain rate for most superplastic materials (flow is non-Newtonian), and even with the strain. A few different mechanisms could be responsible for superplasticity: *e.g.* grain boundary sliding/migration, atomic diffusion and dislocation motion; then if their relative contributions change with strain rate, the strain rate sensitivity would be effected (Kashyap, Arieli and Mukherjee 1985). Deformation-enhanced grain growth may also affect the strain rate sensitivity; understanding how (or if) it does requires identification of the mechanism(s) responsible for this phenomenon so that the kinetics can be properly described. Arieli and Mukherjee (1982) suggest that deformation-enhanced grain growth produces the "threshold," or "plateau" stress which can exist between the diffusional and superplastic creep regimes, characterized by a very small strain rate sensitivity.

Model making in mechanical metallurgy is generally an altogether different undertaking than, for example, model making in physics; see Peierls (1980) for discussion of the latter. Theories are affected by the models from which they have been constructed and therefore need to be developed carefully. Phenomenon considered in mechanical metallurgy are generally the result of complex interactions between elementary constituents of the crystal structure(s) (point, line, and planar defects, solute atoms, phase boundaries) that are induced by thermal and mechanical energy. In most cases models of these phenomenon simplify and/or neglect many processes in order to create a tractable problem. The problem which emerges from such a treatment is not likely to completely resemble the phenomena of interest, even if it succeeds in capturing the "rate limiting step."

Relationships between the flow stress and strain rate are called *constitutive relationships*. Such relationships are of the most value when they are applicable for more than a single strain rate, *e.g.* Ashby and Verrall (1973), and better yet if they give the flow stress as a function of strain by including, for example, the grain growth kinetics. Developing a strain rate and strain dependent constitutive relationship from first principles in a self consistent manner is not a trivial matter. It is not at all clear that there exists a fully developed physical theory (such as "irreversible thermodynamics") available for such an undertaking.

Accommodation mechanisms (*e.g.* atomic diffusion and dislocation motion) for transilatory grain motion (resulting from grain boundary sliding/migration) presumably determine the strain rate sensitivity; but is this the entire story? For example, the work hardening which occurs when metal alloys are plastically deformed at lower homologous temperatures is an immensely complex phenomena arising from multitudinous interactions between dislocations, dislocation arrays, second phase particles, solute atoms, sub-boundaries and grain boundaries. This phenomena cannot be fully understood by describing the properties of single dislocations or dislocation reactions; a different level of description is required, *e.g.* Kuhlmann-Wilsdorf (1987). **The microstructural flow during superplastic deformation is inhomogeneous** (Ashby and Verrall 1973): some grains move more than others (Rai and Grant 1983, Kashyap *et al.* 1985); grains can move in *clumps*, which are aggregates comprised of many grains, as well as individually (Edington, Melton and Cutler 1976, Kashyap *et al.* 1985); some grain boundaries might slide easily, others could be so viscous as to require simultaneous grain rotations (Beeré 1978). The work of Astanin, Kaibyshev and Faizova (1994), and Zelin *et al.* (1994) indicates that the strain rate sensitivity is affected by the tendency for grains to move in clumps; large clumps move at low strain rates and smaller clumps move at higher strain rates. Modelling the motion of small grain groups may therefore not lead to an adequate description of superplasticity.

Ghosh and Raj (1981,1986) and Poirier (1985) emphasize the importance of considering the grain size distribution in developing constitutive relationships, as opposed to only one grain size (the average). Morral and Ashby (1974) model a polycrystalline material as a froth of cells with cellular dislocations and disclinations. Since these defects alter cell shapes and sizes, this model should account for at least some effects of different grain sizes. There is a "dual" lattice to this froth; in three dimensions it is body-centered cubic and in two dimensions it is a lattice with six*fold* symmetry. **Dislocation and disclination motion are inhomogeneous processes.** The extension of the neighbor switching mechanism for superplastic flow provided by cellular defects is developed further here. For example, cellular dislocation reactions are described and utilized to model material behavior; the strain rate sensitivity is affected by the "slip band" spacing, a descriptive measure of the mobile cellular dislocation density.

Cellular dislocation glide results when cells in a froth switch neighbors at the dislocation core, thereby modelling the transilatory grain movements responsible for superplastic flow in a fashion suggestive of McLean's (1970) sequential (inhomogeneous) neighbor switching reaction, as opposed to the homogeneous reactions of Lee (1970), Ashby and Verrall (1973), and Beeré (1976). Sato, Kuribayashi and Horiuchi (1990) use stress-driven cellular dislocation climb as a model for both transilatory grain motion and deformation-enhanced grain growth. Deformation-enhanced grain growth is modelled here with both stress-driven and thermally-activated cellular dislocation climb.

Dislocations are characterized by their Burgers vectors. In a perfect lattice four vectors can be made into a parallelogram; if a dislocation is inserted inside of the parallelogram it opens up; the Burgers vector closes it again. The torsion tensor ($\mathbf{T}$) is a function which, when given the area ($\mathbf{A}$) of a parallelogram surrounding the dislocation, returns the Burgers vector ($\mathbf{b}$): illustratively, $-\mathbf{b} = \int(d\mathbf{b}/d\mathbf{A})d\mathbf{A} = \int \mathbf{T}(\mathbf{A})$. The mathematical "dual" to the torsion tensor is the dislocation density tensor.

A lattice is an example of a "manifold." The study of "manifolds" is differential geometry. The torsion and Riemann curvature tensors are used to take derivatives of functions on "manifolds." The curvature tensor measures the change in a vector that is parallel transported around the periphery of a parallelogram; if this parallelogram is on a Euclidian "manifold" then this change is zero, but if it is on a sphere for example, then there is a change. The mathematical "dual" of the Riemann curvature tensor is the "incompatibility tensor" when the "manifold" is the configuration of a deformed body. The incompatibility tensor contains the compatibility relationships for the strain tensor. Dislocation loops are "compatible" defects, other dislocations, and disclinations, are "incompatible" defects.

Differential geometry is a tool for "counting up space" (Misner, Thorne and Wheeler 1973). This is useful in mechanical metallurgy: If the "manifold" is a crystal lattice, then at low temperatures plastic deformation results from relative motions of assemblies of atoms on opposing sides of slip planes; if the "manifold" is an assemblage of very small grains, then at high temperatures superplastic deformation results from relative grain movements. In both cases pieces of the "manifold" must be measured before and after deformation to determine the strain.

The metric tensor is used in differential geometry to measure distances between points of a "manifold." This tensor is constant for a perfect crystal or froth of uniform cells: all points or cells are equidistant. Grain growth has been simply modelled by considering the rate at which a single "spherical grain" collapses; the size of the grain is taken as the average grain size of the material, a highly simplified "metric." Much more powerful "spherical metrics" are discussed by Onat and Leckie (1988) and De Hoff (1994). The metric tensor of an elastically deformed lattice, or cellular array with a distributed cell size, is spatially dependent. Dislocations and disclinations produce elastic strains in a lattice because the unit cell size, and therefore the metric tensor, becomes spatially dependent by their presence. Analogously, cellular dislocations and disclinations produce "elastic strains" in a froth because the cell size is distributed about some average value and therefore the metric tensor is spatially dependent; these "strains" result because cell boundaries have surface tension. If cell coarsening (the model for grain growth) occurs then the metric tensor is time dependent as well. A spatially and temporally dependent metric tensor for a froth is quite reminiscent of Rhines and Craig's (1974) "structure gradient" model for grain growth.

The compatibility theory of dislocations is developed with exterior calculus at an introductory level. Differential geometry has been used for over forty years to describe aspects of defects in solid materials (Bilby 1960, Kondo 1964) and is still the subject of active research (Venkataraman and Sahoo 1985,1986). Exterior calculus can be viewed as a procedure for doing differential geometry. There is, however, no real introduction to this material aimed towards the background of typical materials scientists.

"Compatibility" of a cellular array corresponds to simple statements, *a la* Rivier (1985), about the distribution of edges amongst the cells. "Conventional" creep changes grain shapes; the cellular array modelling the microstructure is stretched accordingly, and the "dual" lattice deforms "elastically."

The theory of dislocation motion, or lattice plasticity (*e.g.* the Orowan equation), is also developed with exterior calculus. Superplasticity corresponds to flow of a froth via cellular dislocation glide and climb, or to plastic deformation of the "dual" lattice. The two-dimensional neighbor switching mechanisms of superplasticity from Lee (1970), Ashby and Verrall (1973), and Beeré (1976), are analyzed; Beeré's mechanism is "slip-like" for a lattice with six*fold* symmetry. Morral and Ashby's (1974) constitutive relationship for superplastic flow is developed explicitly—with diffusional accommodation as an illustration—and analyzed; it predicts non-Newtonian behavior when the cellular dislocation density increases with strain rate (or flow stress), as they claim.

The constitutive relationship and grain growth kinetics for superplastic flow are illustrated by modelling the behavior exhibited by single phase (Sn-1% Bi) and quasi-single phase (7475 Al) materials (Sherwood and Hamilton 1994). It is suggested that the grain growth kinetics are strain rate dependent: kinetics in one strain rate regime give way to different kinetics when the strain rate is changed. Thermally-activated cellular dislocation climb is suggested as the model for deformation-enhanced grain growth at low strain rates. This mechanism is also used to model the grain growth kinetics during annealing; deformation-enhanced grain growth is attributed to "excess" cellular dislocations produced in the microstructure during flow, an example of a cellular dislocation reaction. Stress-driven cellular dislocation climb is suggested as the model for deformation-enhanced grain growth at high strain rates.

The 7475 Al alloy exhibits "non-ideal" grain growth, *i.e.* the grain growth exponent, n, is much smaller than 1/2, and it decreases with decreasing temperature (Sherwood and Hamilton 1993): the average grain size, $\boldsymbol{d}$, from annealing at temperature T for period t is $\boldsymbol{d} \approx Kt^{n}$, where K increases with temperature, $K = K_{o}^{n}\exp(-\mathrm{n}Q_{GG}/\mathrm{R}T)$; $K_{o} \approx$ *constant*, Q_{GG} is the apparent activation energy for grain growth, and R is the gas constant. During superplastic deformation the grain growth kinetics of 7475 Al are strain, strain rate, and temperature dependent. The grain growth kinetics developed here account for this behavior.